Source acceleration with fine-mesh finite difference and a new convergence criterion in Monte Carlo Inactive Cycles

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1. Introduction

Monte Carlo in the neutronic analysis of reactors refer to a school of stochastic methodologies that seek to obtain a reactor solution by simulating the physical behaviour of a large number of neutrons in the reactor. Such methodologies rely on iteration. They consist of cycles where a neutron source distribution is obtained from the behaviour of simulated neutrons in one cycle, and this is used to determine the starting positions of simulated neutrons in the following cycle. Starting from an arbitrary source distribution, inactive cycles must be conducted to obtain a sufficiently converged fission source distribution before active cycles can be conducted to tally the quantities of interest.

Since the direct simulation of a large number of neutrons is computationally expensive, in the development of Monte Carlo methodologies there is interest in minimising the number of inactive cycles necessary to produce a sufficiently converged neutron source distribution.

The present study explores two methods for reducing the number of inactive cycles. First, a variant to the coarse-mesh finite difference, or CMFD, convergence acceleration method that uses a fine-mesh grid with pin-sized cells instead of a coarse mesh. Second, testing for convergence with the Shannon entropy of the source distribution to dynamically end inactive cycles if sufficient convergence is determined to be obtained early.

2. Methodology

2.1 Partial-Current Coarse-Mesh Finite Difference

The partial-current coarse-mesh finite difference method, or pCMFD, is a method to accelerate the convergence of the neutron source distribution in a high-fidelity iterative scheme, such as Monte Carlo, by coupling it with a low-fidelity deterministic solution [1].

In the pCMFD method, homogenised and group-condensed cross-sections and partial currents are obtained from one cycle of a high-fidelity iterative scheme, these factors are used to construct a low-fidelity deterministic reactor solution, and the fission source distribution of this low-fidelity solution is used to adjust the fission source for the following cycle of the high-fidelity scheme. This coupling is shown in Figure 1.

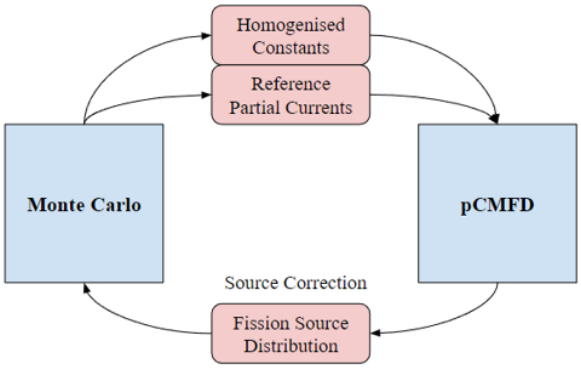

Fig. 1. Convergence acceleration with pCMFD

In pCMFD, the reactor is spatially divided into nodes using a coarse mesh. The one-group neutron balance equation for any given node i adjacent to neighbours j is:

$$\sum_j \frac{A_{ij}}{V_i}\left(J_{ij+} - J_{ij-}\right) + \Sigma_{a,i}\phi_i = \frac{1}{k_{eff}}\nu_i\Sigma_{f,i}\phi_i \qquad (1)$$

where A_{ij} is the surface area of the interface between nodes i and j, V_i is the volume of node i, J_{ij+} and J_{ij-} are the incoming and outgoing partial currents across the interface, and the notation is otherwise conventional.

The partial currents are expressed as:

$$J_{ij+} = \widetilde{D}_{ij}\left(\phi_i - \phi_j\right) + \widehat{D}_{ij}\phi_i \qquad (2)$$

where $\widetilde{D}_{ij}$ is the finite difference method diffusion coefficient and $\widehat{D}_{ij}$ is a correction factor set such that the Eq. 2 reproduces the preliminary Monte Carlo partial current if the preliminary Monte Carlo flux-volume-weighted average fluxes are substituted.

Provisional volume-flux-weighted cross-sections $\Sigma_{a,i}$ and $\nu_i\Sigma_{f,i}$ can be obtained from the Monte Carlo simulation.

Substituting these values and Equation 2 into Equation 1 for each node in the reactor problem produces a system of linear equations. This can be solved for the neutron multiplication factor k_{eff} and the node-average fluxes ϕ_i by the usual iterative methods for eigenvalue problems. In the present study, the stabilised biconjugate gradient method (BiCG-Stab) is used. Once this pCMFD reactor solution is obtained, the pCMFD fission source for each node can be calculated, as $\nu_i\Sigma_{f,i}\phi_{i,pCMFD}$.

The fission source bank for the next iteration of the Monte Carlo simulation is then adjusted. All the neutron sources in a given node are multiplied by a weight such that their total weight equals the node's pCMFD fission source calculated above, as follows:

$$w_{MC,new} = w_{MC,old} \frac{\sum_i w_{pCMFD}}{\sum w_{pCMFD}} \frac{\sum w_{MC,old}}{\sum_i w_{MC,old}} \quad (3)$$

It is conventional for the mesh scheme used in this acceleration method be coarse. That is to say, the nodes are defined such that the radial size of each node matches the radial size of a fuel assembly or equivalent.

However, in principle, the mathematical formulation of the pCMFD acceleration method is not specific to this mesh scheme. It may thus be useful to question whether the magnitude of the convergence acceleration produced by the pCMFD method would not be greater if a different mesh scheme was used. Thus, convergence acceleration via pCMFD using an alternative fine-mesh scheme where each cell in the mesh is radially co-extensive with one fuel pin in driver assemblies or an equivalent amount of space in control assemblies was explored. This variant is referred to as the partial-current fine-mesh finite difference method, or pFMFD. Prior studies suggest that the efficacy of the acceleration may be enhanced for optically thick material if a finer mesh scheme is used [2]. The difference between the two mesh schemes on a hexagonal honeycomb geometry typical of sodium-cooled fast reactors are illustrated in Figure 2.

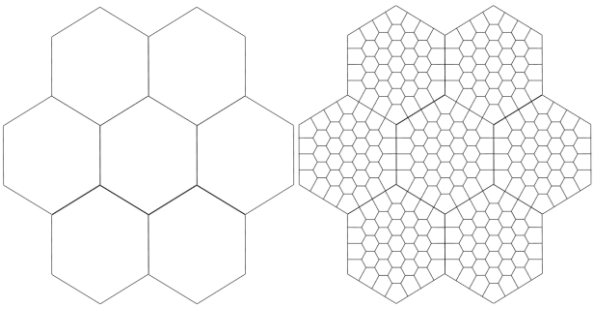

Fig. 2. Conventional pCMFD and pFMFD meshes, radial view

This may, however, introduce stability issues that need to be observed for. Prior studies have found that the pCMFD method is significantly more stable than the older CMFD method based on adjusting for net currents. Fourier analysis revealed that pCMFD acceleration converges regardless of optical thickness except in cases where the mesh used in the acceleration scheme is fine [1], which is exactly the case in the pFMFD method. The stable convergence of the pCMFD/pFMFD deterministic solution is reliant on providing precise cross-sections and partial currents, which may be obtained from the Monte Carlo simulations with a sufficiently high number of particle histories. Previous research using reasoning analogous to Buffon's needle problem has found that in a conventional light water reactor with a neutron crow flight distance 13% of the coarse-mesh width, 5.86 neutrons per node would be necessary to ensure an acceptable low risk, 10^{-5}, of not having Monte Carlo tallies for each pCMFD factor [3]. In the sodium-cooled fast reactor context, with much larger particle flight distances, the number of histories required to guarantee the necessary tallies would be correspondingly lower.

In the present study, source acceleration by pFMFD has been implemented on the iMC code, which is a Monte Carlo neutronics analysis code being developed internally at KAIST [4].

2.2 Shannon Entropy of the Source Distribution

The Shannon entropy is a measure of the amount of semantic information that is contained in a message chosen from a set of messages of differing probabilities and, thus, the semantic information entropy of the probability distribution [5]. It is expressed as

$$H = -\sum_i \{p_i ln(p_i)\} \quad (4)$$

where p_i are the probabilities of some discrete distribution such that $\sum_i p_i = 1$.

Considering the neutron source distribution as a probability distribution, it is possible to obtain a Shannon entropy of the neutron source.

During inactive cycles using the iMC code, this entropy is highest in the initial flat source distribution, then decreases over the inactive cycles to fluctuate around an equilibrium value as the source converges.

Since the convergence of the Shannon entropy reflects the convergence of the fission source, if it is possible to identify the point at which the Shannon entropy reaches sufficient convergence, it would be possible to skip any remaining inactive cycles as unnecessary. However, due to the stochastic cycle-wise fluctuation in Monte Carlo, a conventional relative difference convergence criterion cannot be used.

In this study, an increase in the Shannon entropy from one cycle to the next is presented as one possible convergence test condition. That is to say, if H_n is the Shannon entropy of the neutron source tallied in the nth inactive cycle, and k is the earliest cycle for which

$$H_k > H_{k-1} \quad (5)$$

is true, then it is assumed that after $k + d$ inactive cycles for some small integer d, the fission source has converged sufficiently to begin active cycles with tallying immediately. In this study, $d = 1$ is used.

Such an increase would suggest that the overall downward movement of the entropy over early active cycles as the source distribution converges towards its equilibrium value is sufficiently complete such that random cycle-wise variation caused by the stochastic nature of Monte Carlo can produce a movement in the opposite direction.

Prior research on this subject has generally found that a single-criterion test using the change in the cycle-wise directionality of the Shannon entropy, which is

equivalent to the criterion proposed in this study, is insufficient. It was found that this criterion is very vulnerable to false positives, terminating inactive cycles at a point where convergence has clearly not yet happened [6, 7].

There is nonetheless reason to believe that this single criterion may be sufficient in the present study. Whereas prior research on this subject has accelerated the convergence of its fission source using a fission matrix-based deterministic solution, the present study uses pCMFD/pFMFD acceleration, which is more effective. As the convergence in the fission source is faster, the downwards tendency in the Shannon entropy prior to sufficient source convergence is stronger, and therefore false positives arising from the stochastic variability producing a cycle-wise increase in the Shannon entropy at a point where there is still a downwards tendency in the Shannon entropy should be much rarer.

The iMC code has been extended to allow the simulation to end inactive cycles early before the user-defined number of cycles is complete if there is an increase in the Shannon entropy.

3. Verification

Convergence acceleration with pFMFD and the Shannon entropy convergence criterion were both implemented for a honeycomb geometry on the iMC Monte Carlo code. This code was then tested on a medium-sized sodium-cooled fast reactor problem.

First, one calculation using pFMFD acceleration, one using pCMFD acceleration, and one calculation using neither were performed, to compare the rate of convergence in the neutron multiplication factor and the Shannon entropy during their respective inactive cycles. These calculations were performed with 15 inactive cycles and 15 active cycles.

Second, a calculation using pFMFD acceleration and the Shannon entropy convergence criterion was performed. 15 active cycles were performed. The number of inactive cycles was set at a maximum of 15, but with early termination after one final inactive cycle following the first increase in the Shannon entropy of the source distribution. The tallied results were then compared with reference solutions calculated using 15 inactive cycles, 15 active cycles, and 72.5 million histories per cycle.

The calculations were performed once with 500,000 histories per cycle and once with 2 million per cycle.

3.1 MOX-1000 Reactor Problem

The model core used in the present study is the MOX-1000 reference problem by the Nuclear Energy Agency [8], with some structural elements simplified. It is a three-dimensional model. The active core height is 114.94cm, the assembly pitch 16.2471cm, and the pin pitch 0.913075cm.

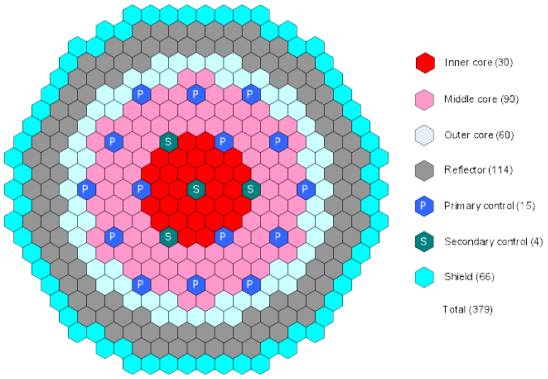

Fig. 3. Radial layout of the MOX-1000 core

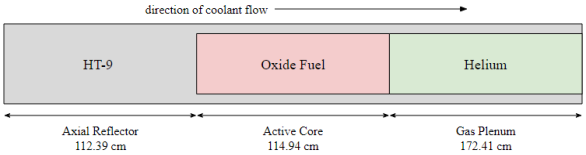

Fig. 4. Axial layout of the MOX-1000 core

The mesh schemes described in the Methodology section was used. Axially, the active core was divided into five axial nodes or cells for the purposes of pCMFD or pFMFD calculations.

4. Results

The results of these calculations are as follows. In the first case, the rates of convergence during inactive cycles were compared. In the second case, the reactor solution tallied in active cycles was examined for bias.

4.1 pCMFD and pFMFD Rates of Convergence

The convergence of the neutron multiplication factor and the Shannon entropy over inactive cycles using pCMFD or pFMFD acceleration are shown in Figures 5 to 8.

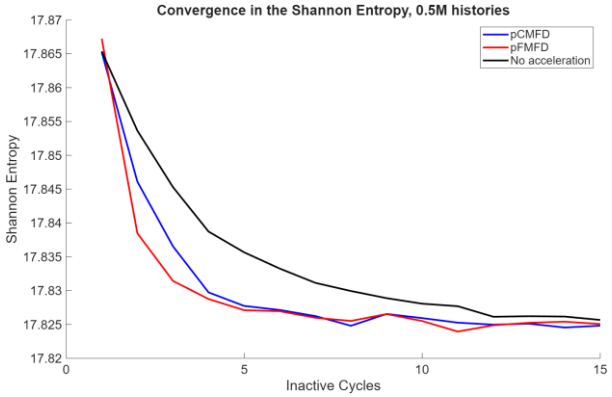

Fig. 5. Shannon entropy, pCMFD in blue, pFMFD in red, 0.5M

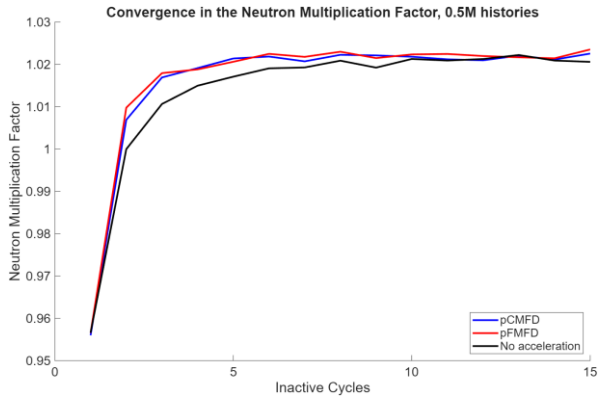

Fig. 6. K-value, pCMFD in blue, pFMFD in red, 0.5M

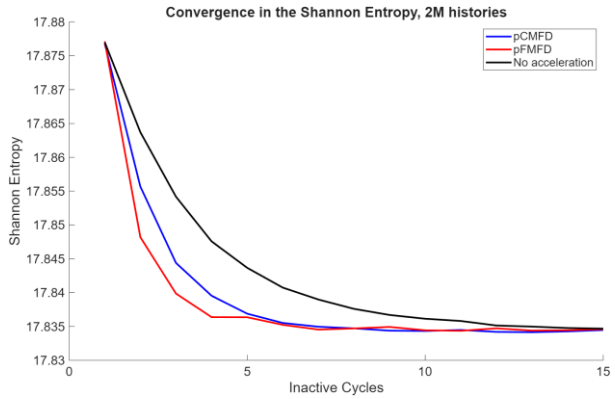

Fig. 7. Shannon entropy, pCMFD in blue, pFMFD in red, 2.0M

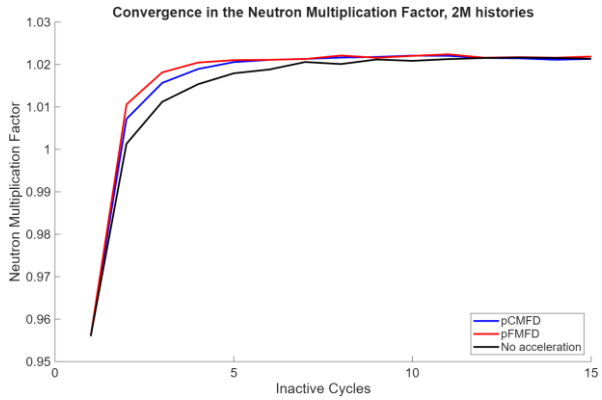

Fig. 8. K-value, pCMFD in blue, pFMFD in red, 2.0M

The effectiveness of pCMFD or pFMFD acceleration is clearly evident. In both cases, the Shannon entropy of the neutron source decreases much faster and the neutron multiplication factor rises much faster with either pCMFD or pFMFD acceleration than it does with neither.

The pFMFD results in particular appear promising. In both cases, the Shannon entropy is significantly lower for acceleration using pFMFD than the same using pCMFD in inactive cycles 2, 3, and 4, indicating that pFMFD acceleration is more effective at accelerating the convergence of the fission source during these early inactive cycles.

The computation time required to construct and solve the pCMFD problem for source convergence acceleration was 0.42 seconds per cycle. For the pFMFD problem, it was 1.57 seconds. The Monte Carlo simulation itself required a mean of 69.80 seconds per cycle in the 500,000 histories per cycle cases and 242.84 seconds per cycle in the 2 million histories per cycle cases. It may therefore be said that the additional computational burden imposed by the pCMFD/pFMFD convergence acceleration schemes is very minor compared to the computation time that may be saved by the resulting reduction in the necessary number of inactive cycles.

4.2 Shannon Entropy Convergence Criterion

In the calculation with pFMFD acceleration and dynamic truncation of inactive cycles, the first increase in the Shannon entropy was observed in the 7th inactive cycle for the 500,000 histories case and in the 6th active cycle for the 2 million histories case.

The neutron multiplication factors and their estimated stochastic uncertainties calculated in the reference calculation and the calculation using the Shannon entropy convergence criterion, here referred to as truncated inactive, are as follows. The uncertainty given for the reference solution is estimated from independent batch calculations. The uncertainty given for the truncated inactive solution is estimated from cycle-wise variance in the tallied value.

Table 1: Neutron multiplication factors and uncertainties

Solution	k-value
Reference	1.021713 (SD 1.6pcm)
Truncated Inactive 0.5M	1.021881 (SD 14.7pcm)
Truncated Inactive 2.0M	1.021708 (SD 9.0pcm)

These values match. The differences between them are well within uncertainties.

The normalised radial power distribution along the axial centre in the reference solution is shown in Figure 9. The relative difference between the truncated inactive solution using 500,000 histories per cycle or the same using 2 million histories per cycle and the reference solution are shown in Figures 10 and 11 respectively.

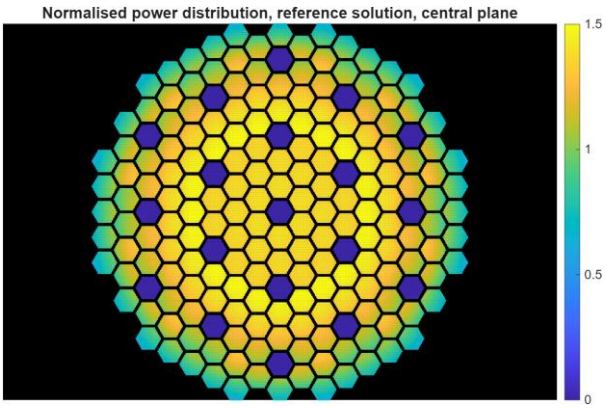

Fig. 9. Normalised power in the reference solution

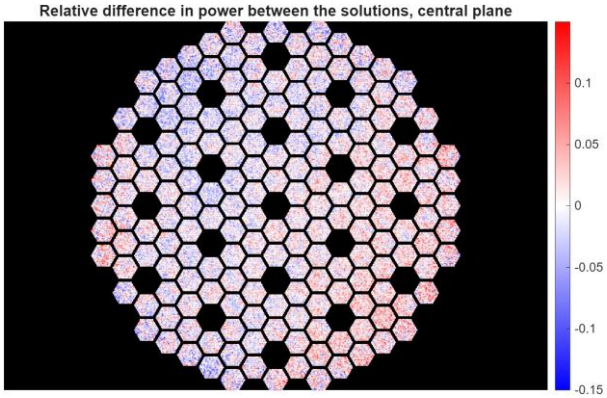

Fig. 10. Relative difference in the power distribution, 0.5M

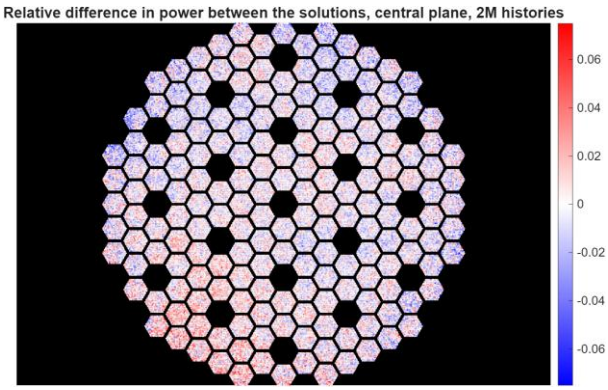

Fig. 11. Relative difference in the power distribution, 2.0M

While a pin-by-pin comparison of the two power distributions reveals some significant differences, this is attributable to the inevitably large stochastic uncertainty in the power distribution of the truncated inactive solution. The differences appear randomly distributed and there is no noticeable systematic bias that may suggest insufficient convergence in the source distribution. 7 or 8 inactive cycles, dynamically set during the Monte Carlo calculations by the Shannon entropy convergence criterion, appears to be sufficient.

5. Conclusions

This study explored the possibility of reducing the computational burden of the Monte Carlo neutronics analysis of reactors in the sodium-cooled fast reactor context by using a fine-mesh scheme for pCMFD source convergence acceleration and dynamically truncating the number of inactive cycles performed based on a Shannon entropy convergence criterion.

The results for the efficacy of pCMFD acceleration with a fine-mesh scheme were promising, with the Shannon entropy of the neutron source distribution decreasing notably faster over the first few inactive cycles if pFMFD acceleration is used relative to if pCMFD acceleration is used. While the computational burden of pFMFD acceleration is larger than that of pCMFD acceleration, it is negligible relative to the total computation time of the Monte Carlo analysis. Further investigation, perhaps using a larger number of independent batches to minimise the effect of stochastic variability on the results, may be warranted.

While firm conclusions regarding the use of a cycle-wise increase in the Shannon entropy as the convergence criterion to dynamically adjust the number of inactive cycles cannot be made from the limited calculations demonstrated in this study, the results are very promising. Dynamically reducing the number of inactive cycles using this criterion did not produce any noticeable bias in the neutron multiplication factor and the source distribution of the resulting solution, indicating that in this particular case this convergence criterion did successfully identify the point at which the source distribution reaches sufficient convergence. Given the results of prior studies and the stochastic nature of our proposed convergence criterion, it will be necessary to repeat the calculations many times to observe the frequency of false positives, if there are any.

ACKNOWLEDGEMENTS

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